

10/513699

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PASSWORD:

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* * * * * Welcome to STN International * * * * *

NEWS	1			Web Page for STN Seminar Schedule - N. America
NEWS	2	OCT	02	CA/CAPLUS enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	3	OCT	19	BEILSTEIN updated with new compounds
NEWS	4	NOV	15	Derwent Indian patent publication number format enhanced
NEWS	5	NOV	19	WPIX enhanced with XML display format
NEWS	6	NOV	30	ICSD reloaded with enhancements
NEWS	7	DEC	04	LINPADOCDB now available on STN
NEWS	8	DEC	14	BEILSTEIN pricing structure to change
NEWS	9	DEC	17	USPATOLD added to additional database clusters
NEWS	10	DEC	17	IMSDRUGCONF removed from database clusters and STN
NEWS	11	DEC	17	DGENE now includes more than 10 million sequences
NEWS	12	DEC	17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS	13	DEC	17	MEDLINE and LMEALINE updated with 2008 MeSH vocabulary
NEWS	14	DEC	17	CA/CAPLUS enhanced with new custom IPC display formats
NEWS	15	DEC	17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS	16	JAN	02	STN pricing information for 2008 now available
NEWS	17	JAN	16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	18	JAN	28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	19	JAN	28	MARPAT searching enhanced
NEWS	20	JAN	28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	21	JAN	28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	22	JAN	28	MEDLINE and LMEALINE reloaded with enhancements
NEWS	23	FEB	08	STN Express, Version 8.3, now available
NEWS	24	FEB	20	PCI now available as a replacement to DPCI
NEWS	25	FEB	25	IFIREF reloaded with enhancements
NEWS	26	FEB	25	IMSPRODUCT reloaded with enhancements
NEWS	27	FEB	29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

<12/04/2007>

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NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 17:17:45 ON 17 MAR 2008

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	1.47	1.47

FILE 'REGISTRY' ENTERED AT 17:22:08 ON 17 MAR 2008
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STRUCTURE FILE UPDATES: 16 MAR 2008 HIGHEST RN 1008362-16-0
DICTIONARY FILE UPDATES: 16 MAR 2008 HIGHEST RN 1008362-16-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

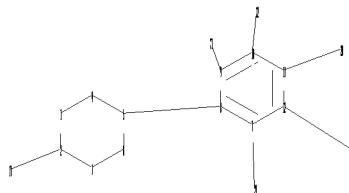
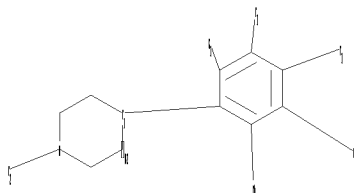
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10581591.str

10/513699



```
chain nodes :
17 19 20 22 23 24
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
2-17 5-8 7-24 9-23 10-22 11-20 12-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-6 2-3 2-17 3-4 4-5 5-6 5-8 7-24 9-23 10-22 11-20 12-19
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12
```

G1:C,N

G2:Cy,Ak,S

G3:X,Cy,Ak,OH,CN,NH2,NO2,H,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 17:CLASS 19:CLASS 20:CLASS 22:CLASS 23:CLASS 24:Atom

L1 STRUCTURE UPLOADED

<12/04/2007>

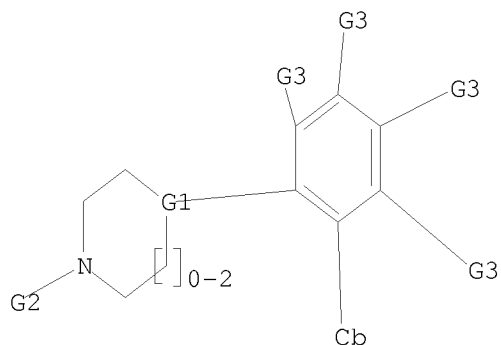
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=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 C,N

G2 Cy,Ak,S

G3 X,Cy,Ak,OH,CN,NH2,NO2,H,O

Structure attributes must be viewed using STN Express query preparation.

=> s 11 full

FULL SEARCH INITIATED 17:23:15 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 13611612 TO ITERATE

1.9% PROCESSED	262703 ITERATIONS	6 ANSWERS
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3.9% PROCESSED	525895 ITERATIONS	11 ANSWERS
----------------	-------------------	------------

6.4% PROCESSED	875810 ITERATIONS	14 ANSWERS
----------------	-------------------	------------

7.2% PROCESSED	977197 ITERATIONS	17 ANSWERS
----------------	-------------------	------------

7.3% PROCESSED	1000000 ITERATIONS	17 ANSWERS
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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.01.11

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 13611612 TO 13611612

PROJECTED ANSWERS: 186 TO 276

L2 17 SEA SSS FUL L1

=>

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

191.24

192.71

FILE 'CAPLUS' ENTERED AT 17:39:39 ON 17 MAR 2008

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FILE COVERS 1907 - 17 Mar 2008 VOL 148 ISS 12
FILE LAST UPDATED: 16 Mar 2008 (20080316/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

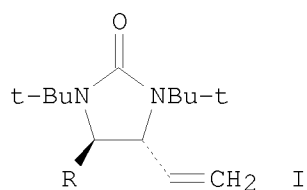
<http://www.cas.org/infopolicy.html>

=> s 12 full
L3 7 L2

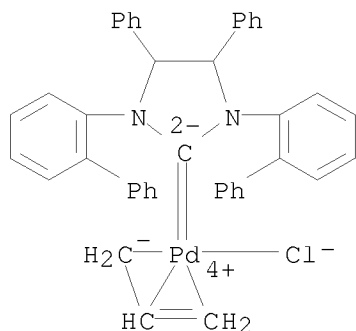
=> d ibib abs hitstr tot

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L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1448274 CAPLUS
DOCUMENT NUMBER: 148:239092
TITLE: Chiral N-Heterocyclic Carbene-Pd(0)-Catalyzed
Asymmetric Diamination of Conjugated Dienes and Triene
AUTHOR(S): Xu, Liang; Shi, Yian
CORPORATE SOURCE: Department of Chemistry, Colorado State University,
Fort Collins, CO, 80523, USA
SOURCE: Journal of Organic Chemistry (2008), 73(2), 749-751
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

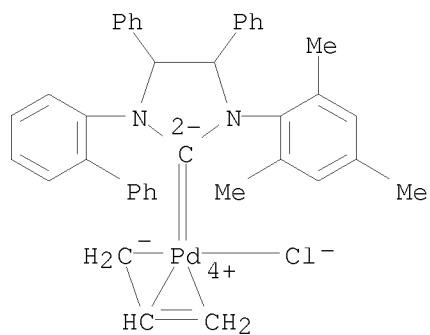


AB Studies show that a variety of conjugated dienes and triene can be enantioselectively diaminated using di-tert-butyl diaziridinone as nitrogen source and chiral N-heterocyclic carbene-Pd(0) complex as catalyst to give diamination products, e.g. I (R = Me, Et, PhCH₂CH₂, n-C₅H₁₁), in good enantioselectivity (62-91% ee) with high regio- and diastereoselectivity.
IT 1006064-38-5P 1006064-42-1P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral N-heterocyclic carbene-Pd catalysts and application to asym. diamination of conjugated dienes and triene using di-tert-butyl diaziridinone)
RN 1006064-38-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



RN 1006064-42-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

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REFERENCE COUNT:

62

THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1364471 CAPLUS

DOCUMENT NUMBER: 148:33768

TITLE: Preparation of bridged aryl piperazines derivatives useful for the treatment of CNS, gastrointestinal and reproductive disorders

INVENTOR(S): Creighton, Christopher John; Ross, Tina Morgan; Reitz, Allen B.; Kordik, Cheryl P.; Paget, Steven

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 122pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

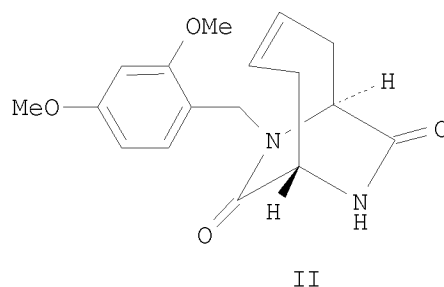
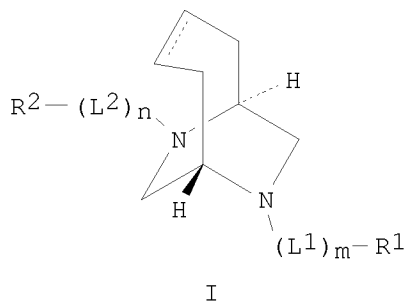
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007137168	A2	20071129	WO 2007-US69256	20070518
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: US 2006-801439P P 20060518

OTHER SOURCE(S): MARPAT 148:33768

GI



AB Title compds. represented by the formula I [wherein m = 0 or 1; L1, L2 = independently -alkyl-, -CH₂-alkenyl-, -CH₂-alkynyl-, etc.; R1, R2 = H, (cyclo)alkyl, aryl, etc.; n = 0 or 1; and pharmaceutically acceptable salts thereof] were prepared as serotonin transport inhibitors and/or modulators of 5HT1A. For example, II was provided in a multi-step

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synthesis starting from the reaction of allylglycine Me ester with 2,4-dimethoxybenzaldehyde. I were tested for radioligand binding to the human 5-HT1A receptor and to human 5-HTT, and for [35S]GTPγS binding of 5-HT1A receptor activation and inhibition. Thus, I and their pharmaceutical compns. are useful for the treatment of depression and related disorders.

IT 959408-27-6P 959408-28-7P 959408-29-8P

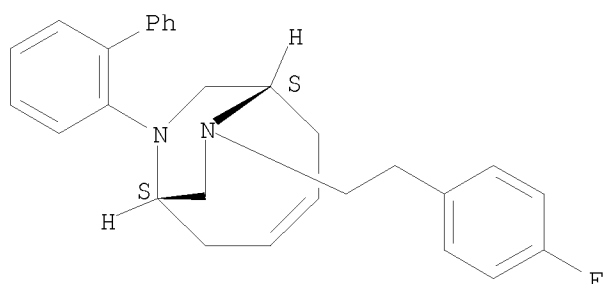
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of bridged aryl piperazines derivs. useful for treatment of CNS, gastrointestinal and reproductive disorders)

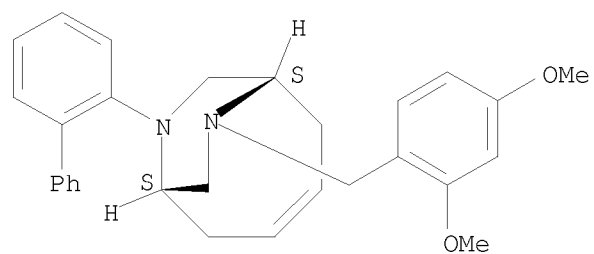
RN 959408-27-6 CAPLUS

CN 7,9-Diazabicyclo[4.2.2]dec-3-ene, 7-[1,1'-biphenyl]-2-yl-9-[2-(4-fluorophenyl)ethyl]-, (1S,6S)- (CA INDEX NAME)

Absolute stereochemistry.



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L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1215849 CAPLUS

DOCUMENT NUMBER: 147:486339

TITLE: Preparation of substituted 4-piperidinylmethyl
phenylmethyl ethers as NK-1 and serotonin transporter
inhibitors

INVENTOR(S): Denhart, Derek J.; Degnan, Andrew P.; Tora, George O.;
Han, Ying; Ramkumar, Rajamani; Ditta, Jonathan L.;
Gillman, Kevin W.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 246pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007121389	A2	20071025	WO 2007-US66682	20070416
WO 2007121389	A3	20080221		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA,
CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB,
GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM,
KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK,
MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

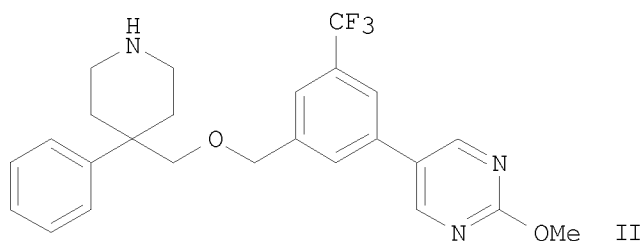
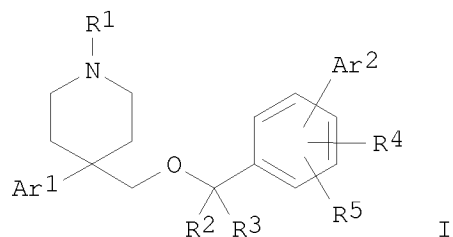
US 2007249607	A1	20071025	US 2007-734809	20070413
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PRIORITY APPLN. INFO.: US 2006-792604P P 20060417

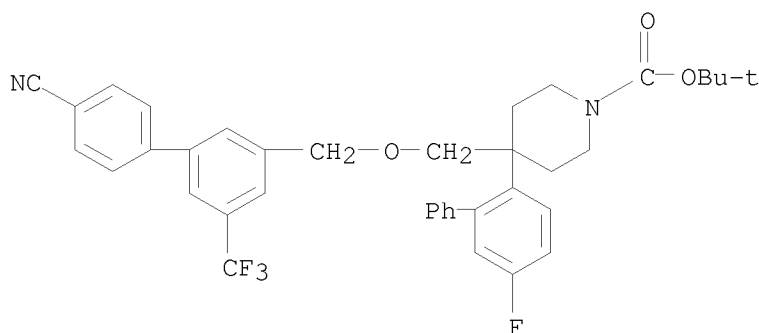
US 2007-734809 A 20070413

OTHER SOURCE(S): MARPAT 147:486339

GI



- AB The title compds. I [R1 = H, alkyl, cycloalkyl, CH2Ph; R2, R3 = H or alkyl; R4, R5 = H, alkyl, haloalkyl, etc.; Ar1 = (un)substituted Ph or pyridinyl; Ar2 = (un)substituted Ph, naphthyl, furanyl, etc.], useful in treating disorders associated with an excess or imbalance of tachykinins or serotonin or both, were prepared. E.g., a multi-step synthesis of II, starting from 4-phenyl-4-piperidinecarboxylic acid p-methylbenzenesulfonate, was given. II showed IC50 of 0.01-100 nM when tested in NK-1 binding assay and in serotonin transporter binding assay. Pharmaceutical composition comprising the compound I is disclosed.
- IT 954123-38-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of substituted 4-piperidylmethyl phenylmethyl ethers as NK-1 and serotonin transporter inhibitors)
- RN 954123-38-7 CAPLUS
- CN 1-Piperidinecarboxylic acid, 4-[[[4'-cyano-5-(trifluoromethyl)[1,1'-biphenyl]-3-yl]methoxy]methyl]-4-(5-fluoro[1,1'-biphenyl]-2-yl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



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<12/04/2007>

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L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1213121 CAPLUS

DOCUMENT NUMBER: 147:502389

TITLE: Preparation of diketo-piperazine and piperidine derivatives as antiviral agents

INVENTOR(S): Wang, Tao; Kadow, John F.; Zhang, Zhongxing; Yin, Zhiwei; Meanwell, Nicholas A.; Regueiro-Ren, Alicia; Swidorski, Jacob; Han, Ying; Carini, David J.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: U.S. Pat. Appl. Publ., 277pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2007249579	A1	20071025	US 2007-733283	20070410
WO 2007127635	A2	20071108	WO 2007-US66700	20070416
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.:	US 2006-794700P	P	20060425
	US 2006-794703P	P	20060425
	US 2007-733283	A	20070410

OTHER SOURCE(S): MARPAT 147:502389

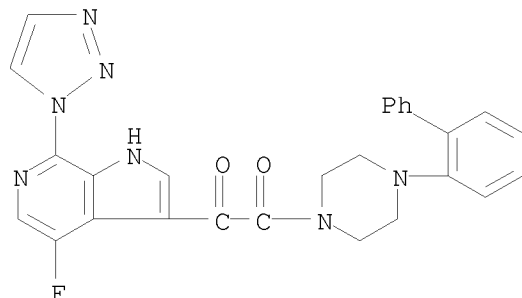
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

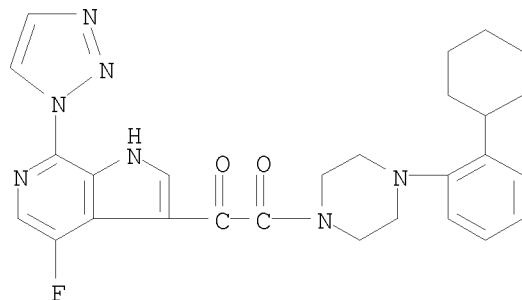
AB Title compds. I [Ring A = (un)substituted 6-membered aryl or nitrogen heteroaryl; R1 = H, alkyl or fluoroalkyl; R2 = H; R3-10 independently = H or (un)substituted alkyl; Y = (un)substituted Ph, monocyclic heteroaryl, bicyclic aryl, etc.; Z = alkyl, alkoxy, cycloalkyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as antiviral agents. Thus, e.g., II was prepared by Friedel-Craft acylation of 7-bromo-4-fluoro-1H-pyrrolo[2,3-c]pyridine with Me chlorooxoacetate followed by amidation with 1-(1-phenyl-1H-tetrazol-5-yl)piperazine (preparation given). In particular, the disclosure is concerned with diketo piperazine and piperidine derivs. that possess unique antiviral activity. EC50 values were determined for I with results reported in ranges with one group possessing EC50 values of $\leq 0.5 \mu\text{M}$ and the other as $> 0.5 \mu\text{M}$. More particularly, the present disclosure relates to compds. useful for the treatment of HIV and AIDS.

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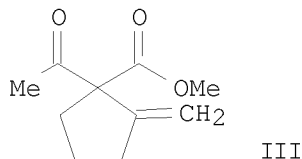
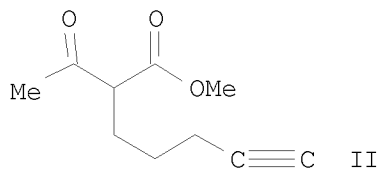
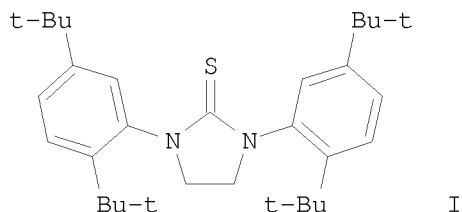
IT 955045-27-9P 955045-64-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of diketo-piperazine and piperidine derivs. as antiviral
agents)
RN 955045-27-9 CAPLUS
CN 1,2-Ethanedione, 1-(4-[1,1'-biphenyl]-2-yl-1-piperazinyl)-2-[4-fluoro-7-
(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]- (CA INDEX NAME)



RN 955045-64-4 CAPLUS
CN 1,2-Ethanedione, 1-[4-(2-cyclohexylphenyl)-1-piperazinyl]-2-[4-fluoro-7-
(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]- (CA INDEX NAME)



L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:1026919 CAPLUS
 DOCUMENT NUMBER: 147:502036
 TITLE: Bulky thioureas as new ligands for gold(I)-catalyzed cyclization of acetylenic 1,3-dicarbonyl compounds
 AUTHOR(S): Pan, Jie-Hui; Yang, Min; Gao, Qiang; Zhu, Nian-Yong; Yang, Dan
 CORPORATE SOURCE: Department of Chemistry, The University of Hong Kong, Hong Kong, Peop. Rep. China
 SOURCE: Synthesis (2007), (16), 2539-2544
 CODEN: SYNTBF; ISSN: 0039-7881
 PUBLISHER: Georg Thieme Verlag
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB We illustrate the first use of bulky N,N'-disubstituted cyclic thioureas, e.g. I, as ligands for gold(I) catalysis. X-ray crystal structures of the thiourea-gold(I) complexes presented important information about the nature of the complexation. These complexes were found to be active catalysts for the cyclization of 1,3-dicarbonyl compds. with alkynes (Conia-ene reaction). Various acetylenic 1,3-dicarbonyl compds. underwent cycloisomerization to give mono- and bicyclic olefinic cyclopentanes in the presence of one mol% of a thiourea-gold(I) chloride complex and silver triflate. E.g., gold(I)-catalyzed cyclization of acetylenic 1,3-dicarbonyl compound II gave 96% cyclopentane derivative III.

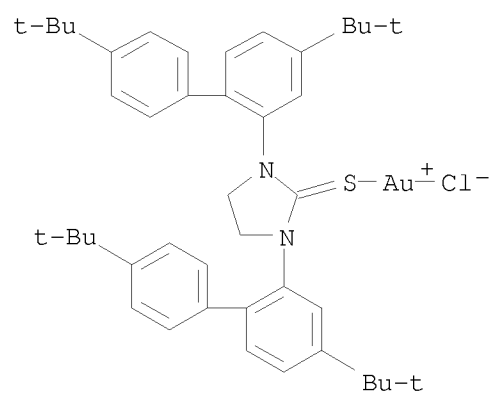
IT 955083-84-8P

RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation);
 PREP (Preparation); USES (Uses)
 (bulky thioureas as ligands for gold(I)-catalyzed cyclization of
 acetylenic 1,3-dicarbonyl compds.)

RN 955083-84-8 CAPLUS

CN Gold, [1,3-bis[4,4'-bis(1,1-dimethylethyl)[1,1'-biphenyl]-2-yl]-2-imidazolidinethione-κS2]chloro- (CA INDEX NAME)

10/513699



REFERENCE COUNT:

31

THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

<12/04/2007>

Erich Leese

L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:806254 CAPLUS

DOCUMENT NUMBER: 147:385945

TITLE: Structure-Activity Relationship Study on
N-(1,2,3,4-Tetrahydronaphthalen-1-yl)-4-aryl-1-
piperazinehexanamides, a Class of 5-HT7 Receptor
Agents. 2AUTHOR(S): Leopoldo, Marcello; Lacivita, Enza; Contino,
Marialessandra; Colabufo, Nicola A.; Berardi,
Francesco; Perrone, RobertoCORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi
di Bari, Bari, 70125, ItalySOURCE: Journal of Medicinal Chemistry (2007), 50(17),
4214-4221

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:385945

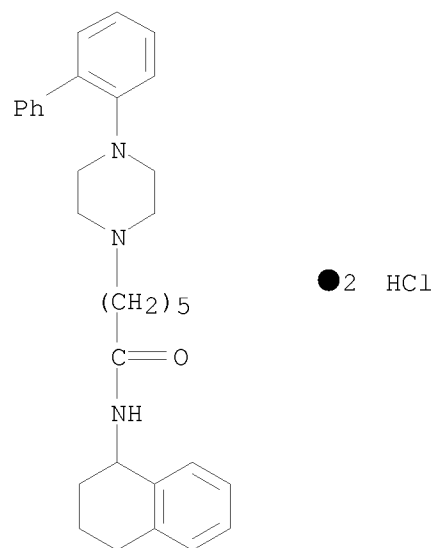
AB Here the authors report the synthesis of N-(1,2,3,4-tetrahydronaphthalen-1-yl)-4-aryl-1-piperazinehexanamides 16-29 that were designed to elucidate both structure-affinity and -activity relations for the 5-HT7 receptor, by targeting the substituent in 2-position of the aryl linked to the piperazine ring. The affinities of 16-29 for 5-HT7, 5-HT1A, 5-HT2A, and D2 receptors were assessed by radioligand binding assays. The intrinsic activities at the 5-HT7 receptor of the most potent compds. were determined. Substituents covering a wide range of electronic, steric, and polar properties were evaluated, revealing a key role on 5-HT7 receptor affinity and intrinsic activity. Certain lipophilic substituents (SCH3, CHMe2, NMe2, CH3, Ph) led to high-affinity agonists, whereas OH and NHCH3 substituents switched intrinsic activity toward antagonism. 4-[2-(1-Methylethyl)phenyl]-N-(1,2,3,4-tetrahydronaphthalen-1-yl)-1-piperazinehexanamide (19), 4-(2-diphenyl)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)-1-piperazinehexanamide (21), and 4-(2-dimethylaminophenyl)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)-1-piperazinehexanamide (22) were identified as potent 5-HT7 receptor agonists ($K_i = 0.13\text{--}1.1\text{ nM}$, $EC_{50} = 0.90\text{--}1.77\text{ }\mu\text{M}$), showing selectivity over 5-HT1A, 5-HT2A, and D2 receptors.

IT 950685-64-0P, 4-(Biphenyl-2-yl)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)-1-piperazinehexanamide dihydrochloride
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and structure-activity relationship for N-(1,2,3,4-tetrahydronaphthalen-1-yl)-4-aryl-1-piperazinehexanamides as a class of selective 5-HT7 receptor agents)

RN 950685-64-0 CAPLUS

CN 1-Piperazinehexanamide, 4-[1,1'-biphenyl]-2-yl-N-(1,2,3,4-tetrahydro-1-naphthalenyl)-, hydrochloride (1:2) (CA INDEX NAME)

10/513699



REFERENCE COUNT:

40

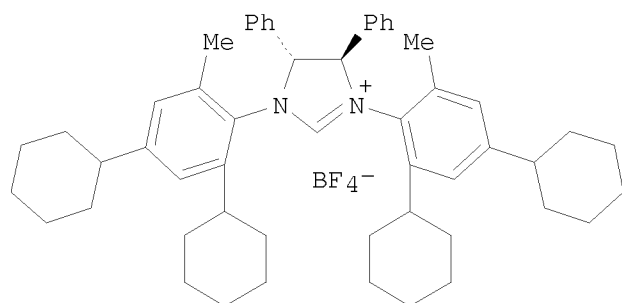
THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

<12/04/2007>

Erich Leese

10/513699

L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:800288 CAPLUS
DOCUMENT NUMBER: 147:343686
TITLE: New N-Heterocyclic Carbene Ligand and Its Application
in Asymmetric Nickel-Catalyzed Aldehyde/Alkyne
Reductive Couplings
AUTHOR(S): Chaulagain, Mani Raj; Sormunen, Grant J.; Montgomery,
John
CORPORATE SOURCE: Department of Chemistry, University of Michigan, Ann
Arbor, MI, 48109-1055, USA
SOURCE: Journal of the American Chemical Society (2007),
129(31), 9568-9569
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:343686
GI



I

AB A new chiral N-heterocyclic carbene ligand (I) has been prepared and examined in nickel-catalyzed, asym. reductive couplings of aldehydes and alkynes. In comparison with related structures that have been largely examined in asym. ring-closing metathesis reactions, the new ligand provides superior yields and enantioselectivities in the nickel-catalyzed reductive couplings. The scope of asym. couplings in intermol. variants as well as a 14-membered macrocyclization is illustrated.

IT 948892-06-6P 948892-13-5P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

(preparation of chiral imidazolium ligands via coupling of chiral diamines with aryl or cyclohexyl bromide followed by cyclization for use in asym. coupling reactions)

RN 948892-06-6 CAPLUS

CN 1H-Imidazolium, 1,3-bis(2-cyclohexylphenyl)-4,5-dihydro-4,5-diphenyl-,
(4R,5R)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

CRN 948892-05-5

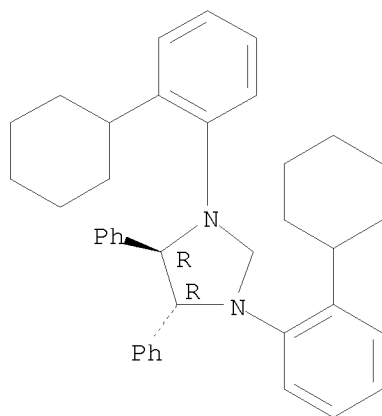
CMF C39 H43 N2

<12/04/2007>

Erich Leese

10/513699

Absolute stereochemistry.



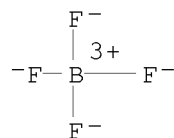
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



RN 948892-13-5 CAPLUS

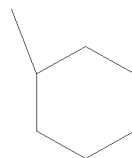
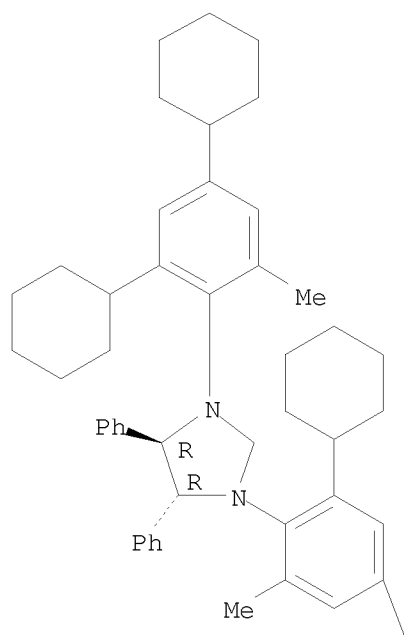
CN 1H-Imidazolium, 1,3-bis(2,4-dicyclohexyl-6-methylphenyl)-4,5-dihydro-4,5-diphenyl-, (4R,5R)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

CRN 948892-12-4

CMF C53 H67 N2

Absolute stereochemistry.



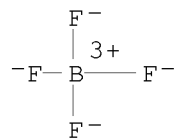
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



IT 948892-29-3

RL: CAT (Catalyst use); USES (Uses)

10/513699

(stereoselective preparation of alkenyl silyl ethers via nickel catalyzed coupling of aldehydes with alkynes in the presence of triethylsilane and chiral imidazolium ligands)

RN 948892-29-3 CAPLUS

CN 1H-Imidazolium, 1,3-bis(2,4-dicyclohexyl-6-methylphenyl)-4,5-dihydro-4,5-diphenyl-, (4S,5S)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

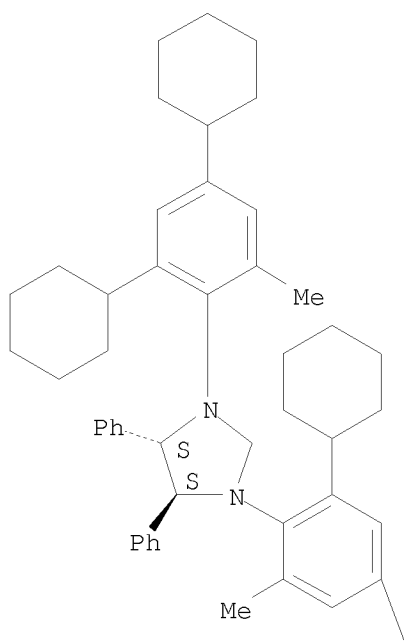
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CRN 948892-28-2

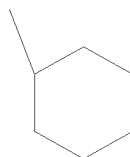
CMF C53 H67 N2

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

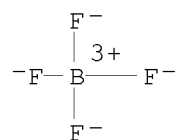
CRN 14874-70-5

<12/04/2007>

Erich Leese

10/513699

CMF B F4
CCI CCS



REFERENCE COUNT:

30

THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/513699

=> d his

(FILE 'HOME' ENTERED AT 17:17:45 ON 17 MAR 2008)

FILE 'REGISTRY' ENTERED AT 17:22:08 ON 17 MAR 2008

L1 STRUCTURE UPLOADED

L2 17 S L1 FULL

FILE 'CAPLUS' ENTERED AT 17:39:39 ON 17 MAR 2008

L3 7 S L2 FULL

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

40.07

232.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-5.60

-5.60

STN INTERNATIONAL LOGOFF AT 17:41:47 ON 17 MAR 2008